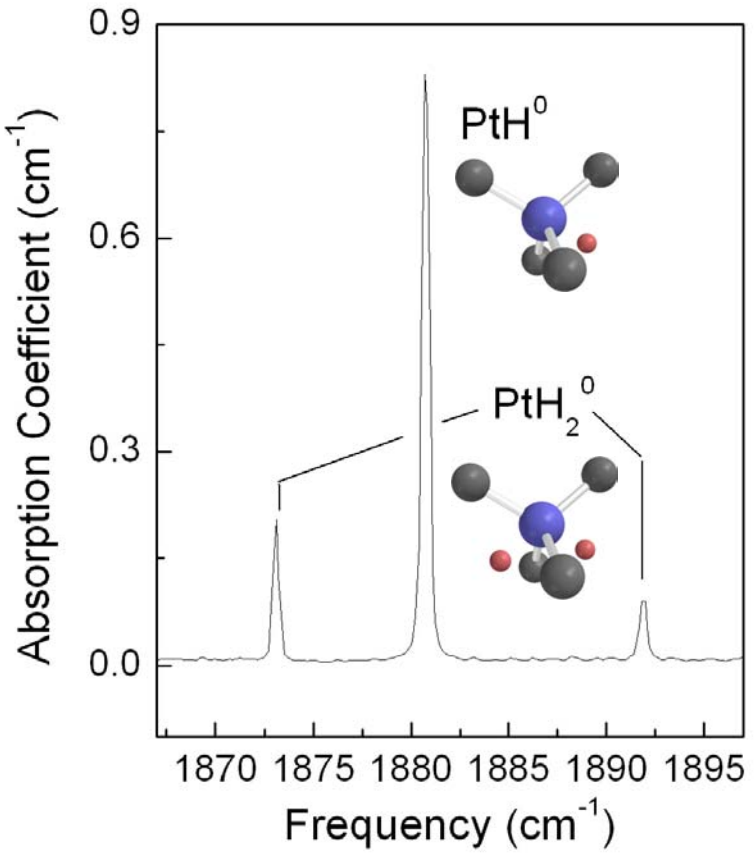
Structures and Properties of Hydrogen-Containing Defects in Semiconductors

Michael Stavola, Lehigh University, DMR-0108914

Hydrogen is an important impurity in semiconductors and is the subject of intense experimental and theoretical study because of its fascinating fundamental properties and its impact on semiconductor technology. H can be introduced into semiconductors to passivate unwanted defects or to take part in novel processes. For example, the efficiencies of solar cells fabricated from multicrystalline Si are improved by the introduction of H. H can also be introduced into semiconductors unintentionally where it affects the control of the electrical properties of the material. In the present grant, the structures and properties of important H-containing defects in semiconductors are studied by vibrational spectroscopy.

Previously, it has not been possible to detect H introduced into Si by methods commonly used to fabricate solar cells because of its low concentration. Our work on the transition-metal-H complexes in Si has led us to develop a sensitive new method to study the introduction of H into Si. We use IR spectroscopy coupled with Pt impurities introduced into Si test samples to act as model traps for H. The Pt-H complexes (right) can be sensitively detected to determine the concentration of H. This novel method to sensitively detect H in Si, based on the results of fundamental studies supported by this grant, is providing new microscopic information about processes used to hydrogenate Si solar cells.



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Students in this program learn about semiconductors, crystal defects and the optical properties of materials, providing a strong foundation for careers in education or industrial R&D. Four graduate students and three undergraduate students (six of whom are women) have performed all of the experimental work supported by this grant. Elinor Chen received her Ph.D. in July, 2002 and is presently a Research Professional in the Dept. of Radiology at the Univ. of Chicago. Another student will defend her Ph.D. in Nov., 2003. Two additional graduate students are studying interstitial H_2 in Si and H in III-N-V alloys and in wide bandgap semiconductors by vibrational spectroscopy in conjunction with applied uniaxial stresses.

Undergraduate students who have worked on this project are part of a long-standing Research Experiences for Undergraduates program that is conducted each summer at Lehigh Univ. Highly qualified students are recruited nationwide to help expose students, often from small colleges, to university-level research programs. Marjan Saboktakin (upper right, Physics and EE, Lehigh Univ.) has studied H in ZnO, an important wide bandgap semiconductor, by IR spectroscopy during summer 2003. Marsha Logan (lower right, Physics, Benedict College) has worked on molecular models to explain the vibrational properties of impurities in semiconductors studied experimentally by the present grant under the supervision of W.B. Fowler (Lehigh Univ.) during summer 2003.